Amendments to the Specification:

Please replace the reference to Figure 6 under Description of the Drawings on page 21 with the following amended description:

~~Figure 6~~ Figures 6A through 6C ~~shows~~ show three molecular structures numbered and marked in accordance with the topomeric alignment rule.

Please replace the reference to Figure 7 under Description of the Drawings on page 21 with the following amended description:

~~Figure 7~~ Figures 7(a) through 7(t) are ~~is~~ a complete set of Patterson plots for the twenty data sets used for the validation studies of the topomeric CoMFA descriptor.

Please replace the reference to Figure 8 under Description of the Drawings on page 21 with the following amended description:

~~Figure 8~~ Figures 8A and 8B show ~~shows~~ the two scatter plots displaying the relation between X^2 values and their corresponding density ratio values for the tested metrics over the twenty random data sets.

Please replace the reference to Figure 9 under Description of the Drawings on page 21 with the following amended description:

~~Figure 9~~ Figures 9A through 9C show ~~shows~~ the graphs of the Tanimoto similarity measure vs. the pairwise frequency of active molecules for 18 groups examined from Index Chemicus.

Please replace the reference to Figure 10 under Description of the Drawings on page 21 with the following amended description:

~~Figure 10~~ Figures 10A and 10B show ~~shows~~ a Patterson plot of the Cristalli data set using only those values which would have been used for a Tanimoto sigmoid plot of the same data set alongside a Patterson plot of the complete data set.

Please replace the reference to Figure 11 under Description of the Drawings on page 21 with the following amended description:

~~Figure 11~~ Figures 11A through 11C are schematics ~~is a schematic~~ of the combinatorial screening library design process.

Please replace the title of the invention appearing on page 1 with the following amended title:

Computer-implemented method of merging libraries of molecules using validated molecular structural descriptors and neighborhood distances to maximize diversity and minimize redundancy.